Cosmic Hydrogen Was Significantly Neutral a Billion Years After the Big Bang

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The ionization fraction of cosmic hydrogen, left over from the big bang, provides crucial fossil evidence for when the first stars and quasar black holes formed in the infant universe. Spectra of the two most distant quasars known[1] show nearly complete absorption of photons with wavelengths shorter than the Lyα transition of neutral hydrogen, indicating that hydrogen in the intergalactic medium (IGM) had not been completely ionized at a redshift $z \sim 6.3$, about a billion years after the big bang. Here we show that the radii of influence of ionizing radiation from these quasars imply that the surrounding IGM had a neutral hydrogen fraction of tens of percent prior to the quasar activity, much higher than previous lower limits [1,2] of $\sim 0.1\%$. When combined with the recent inference of a large cumulative optical depth to electron scattering after cosmological recombination from the WMAP data[3], our result suggests the existence of a second peak in the mean ionization history, potentially due to an early formation episode of the first stars.

The detection of a Lyα emitting galaxy at $z \sim 6.56$ led to the claim that the IGM must already be highly ionized at that redshift[4]. However, it was later shown[5] that the presence of a small ionized region around the galaxy and broadening of the Lyα line,

would allow detection of the line feature in a fully neutral IGM. Luminous quasars offer an alternative probe of the IGM and have higher luminosities, allowing acquisition of higher quality spectra. The spectra[6,7] of SDSS J1030+0524 at $z = 6.28$ and SDSS J1148+5251 at $z = 6.41$ show transmitted flux down to wavelengths corresponding to the Lyα resonance of hydrogen at $z \sim 6.20$ and $z \sim 6.32$ respectively, even though no flux is detected at somewhat greater distances from the quasars[7]. These redshift displacements correspond to velocity shifts of order ~ 3300 km s^{-1}, and imply ionized regions surrounding the quasars with observed physical radii of $R_{\rm obs} = 4.5$ Mpc and 4.7 Mpc, respectively. The inference is robust since high ionization broad-lines typically have velocity offsets from the true quasar redshift[8] of only $\lesssim 1000$ km s^{-1}.

We model the evolution of a fully ionized region (the so-called *Strömgren sphere*) around a quasar that emits UV photons into a partially neutral IGM. Prior to the overlap phase of ionized hydrogen (H II) regions that signals the end of the reionization epoch[9], galaxies generated their own small ionized regions filling a fraction of the IGM volume around the quasar. We define the neutral fraction, $x_{\rm HI}$, to be the mean fraction of hydrogen atoms (in a representative volume of the low-density IGM) that remain neutral prior to the quasar activity, and assume $x_{\rm HI}$ outside the Strömgren sphere to remain constant during its expansion. Since the luminosity of a bright quasar is much larger than the stellar luminosity of neighboring galaxies, a fully ionized quasar bubble expands into a partially ionized IGM composed of isolated H II regions.

Even for the deepest available spectra, with lower limits on the Lyα (*Gunn-Peterson*[10]) optical depth of $\tau_{\rm GP} \gtrsim 26$, the IGM need only have a neutral fraction of $\sim 10^{-3}$ in order to produce the observed absorption blueward of Lyα[1]. However, the value of $R_{\rm obs} \sim 4.5$Mpc may be used to constrain larger values of the neutral fraction in the range $0.001 \leq x_{\rm HI} \leq 1.0$. In the early expansion phase, the dependence of the

physical radius of the Strömgren sphere, $R_{\rm p}$, on the quasar age[1,11], $t_{\rm age}$, may be crudely approximated as $R_{\rm p} \sim 7x_{\rm HI}^{-1/3}\left[t_{\rm age}/10^7{\rm yr}\right]^{1/3}{\rm Mpc}$, given the production rate of ionizing photons that is characteristic of SDSS J1148+5251 and SDSS J1030+0524. Clearly, the Strömgren sphere grows larger when embedded in an IGM with a small neutral fraction. Defining $R_{\rm max}$ to be the maximum radius achieved in a fully neutral IGM by the end of the quasar lifetime, $t_{\rm lt}$, the resulting a priori probability distribution is, $dP/dR_{\rm p}|_{x_{\rm HI}} = 3x_{\rm HI}R_{\rm p}^2/R_{\rm max}^3$ for $R_{\rm p} < R_{\rm max}x_{\rm HI}^{-1/3}$. In addition, the neutral fraction must be smaller than $x_{\rm max} = \min\left(\left[t_{\rm lt}/10^7{\rm years}\right]\left[R_{\rm obs}/7{\rm Mpc}\right]^{-3}, 1\right)$ to allow the growth of the sphere to $R_{\rm obs}$ within $t_{\rm lt}$. Using a flat logarithmic prior for $x_{\rm HI}$, we find the cumulative a posteriori probability distribution, $P(<x_{\rm HI}) = \min(x_{\rm HI}, x_{\rm max})/x_{\rm max}$. Since estimates of quasar lifetimes[12] are bracketed in the range $10^6 - 10^8$ years, we get $x_{\rm max} \sim 1$ and conclude that $x_{\rm HI} \gtrsim 0.1$ (0.01) with 90% (99%) confidence.

To better quantify this simple argument, we write the general equation for the relativistic expansion of the *co-moving* radius $[R = (1+z)R_{\rm p}]$ of the quasar H II region[1] in an IGM with a neutral filling fraction $x_{\rm HI}$ (fixed by other ionizing sources),

$$\frac{dR}{dt} = c(1+z)\left[\frac{F_\gamma \dot{N}_{\rm ion} - \alpha_{\rm B} C F_{\rm m} x_{\rm HI}\left(\bar{n}_0^{\rm H}\right)^2 (1+z)^3\left(\frac{4\pi}{3}R^3\right)}{F_\gamma \dot{N}_{\rm ion} + 4\pi R^2 (1+z)\, c F_{\rm m} x_{\rm HI}\bar{n}_0^{\rm H}}\right], \tag{1}$$

where c is the speed of light, $\bar{n}_0^{\rm H}$ is the mean number density of protons at $z = 0$, $\alpha_{\rm B} = 2.6\times10^{-13}{\rm cm^3 s^{-1}}$ is the case-B recombination coefficient at the characteristic temperature of 10^4K, and $\dot{N}_{\rm ion}$ is the rate of ionizing photons crossing a shell at the radius of the H II region at time t. We use the distribution derived from numerical simulations for the over-densities in gas clumps[13], and calculate the mean free path $d(\Delta_{\rm c})$ for ionizing photons[13,14]. Following Barkana & Loeb[14], we then find the critical overdensity $(\Delta_{\rm c})$ at which a fraction $F_\gamma \equiv 0.5 = \exp\left[-R_{\rm p}/d(\Delta_{\rm c})\right]$, of photons emitted do not encounter an overdensity larger than $\Delta_{\rm c}$ within the H II region. We also compute the mass fraction $F_{\rm m}$ (~ 1) of gas within $R_{\rm p}$ that is at over-densities lower than $\Delta_{\rm c}$. Finally, we calculate the

clumping factor in the ionized regions, $C(R) \equiv \langle\Delta^2\rangle/\langle\Delta\rangle^2$, where the angular brackets denote an average over all regions with $\Delta < \Delta_c$. For $x_{\rm HI} = 1$ and $dR_p/dt \ll c$, equation (1) reduces to its well-known form[11,15–17]. The expansion of the quasar Strömgren sphere would change in an overdense region of the IGM. However the density contrast due to infall has been shown[14] to be small ($\sim 1\%$) on scales of several Mpc around the massive hosts of the bright SDSS quasars at $z \sim 6$. Numerical experiments showed our results to be insensitive to infall. The emission rate of ionizing photons $\dot{N}_{\rm ion}$ in equation (1) is computed at $t' = t - t_{\rm delay}$ to account for the finite light travel time between the source and the ionization front. The delay $t_{\rm delay}$ is derived from the relation $R = \int_{t_R - t_{\rm delay}}^{t_R} cdt'\,[1 + z(t')]$, where t_R is the time when the photon crosses the co-moving radius R. The use of the Telfer et al.[18] spectral template implies $\dot{N}_{\rm ion} = 6.5 \times 10^{57}{\rm s}^{-1}$ for SDSS J1030+0524 and $\dot{N}_{\rm ion} = 10.0 \times 10^{57}{\rm s}^{-1}$ for SDSS J1148+5251, while the template of Elvis et al.[19] implies lower values of $\dot{N}_{\rm ion} \sim 1.3 \times 10^{57}{\rm s}^{-1}$ and $\dot{N}_{\rm ion} \sim 2.0 \times 10^{57}{\rm s}^{-1}$, respectively[1].

Our model for the evolution of the Strömgren sphere includes the quasar formation history. We compute the time dependent ionizing flux governed by black-hole growth through accretion and mergers. Following the observational inference that the relation between bulge velocity dispersion and black hole mass $M_{\rm bh}$ does not evolve with redshift[20], we extrapolate the present-day $M_{\rm bh}$–$M_{\rm halo}$ relation[21] using the dependence of virial velocity on redshift[9] to obtain $M_{\rm halo} = 1.5 \times 10^{12} M_\odot\,(M_{\rm bh}/10^9 M_\odot)^{3/5}\,[(1+z)/7]^{-3/2}$. The luminosities of the SDSS quasars imply black-hole masses of $\sim 2 \times 10^9 {\rm M}_\odot$ accreting at their Eddington rate[6], leading to inferred host dark-matter halos of $M_{\rm halo} \sim 2 \times 10^{12}{\rm M}_\odot$. The inference of such a massive halo at this early epoch is supported by the signature of gas infall in the spectra of high redshift quasars[14], and the inference of a large molecular mass and velocity width in the host galaxy of SDSS J1148+5251[7].

We begin with two dark-matter halos of comparable mass M_1 and M_2 that merge to

form the host dark-matter halo with a mass $M_{\rm halo} = (M_1 + M_2)$ at a redshift corresponding to one quasar lifetime prior the observed redshift, and construct merger trees for each of the progenitor halos using the algorithm described by Volonteri et al.[22]. We use the $M_{\rm bh}$–$M_{\rm halo}$ relation to find the mass of the black-hole at the center of each dark-matter halo in the merger tree. When there is a major merger (having a progenitor mass ratio < 2), we assume that the black-holes merge and that the accretion of the mass deficit relative to the $M_{\rm bh}$–$M_{\rm halo}$ relation produces the limiting Eddington luminosity with a radiative efficiency of $\epsilon = 10\%$. The resulting quasar lifetime is $t_{\rm lt} = 4 \times 10^7 (\epsilon/0.1) \ln \left[M_{\rm halo}^{5/3} / (M_1^{5/3} + M_2^{5/3}) \right]$ years. The ionizing photon emission rate $\dot{N}(t)$ is taken to have an exponential time dependence, $\dot{N}_{\rm ion}(t) = \dot{N}_0 e^{-t/t_{\rm lt}}$, with $\dot{N}_0 \propto M_{\rm bh}$. We assume that all quasar episodes in the merger tree contribute to the volume of the observed Strömgren sphere, which is centered on the most massive halo in the tree. A similar prescription for quasar activity was shown to be consistent with the observed number counts of high redshift quasars[22]. For a major merger resulting in the observed quasar activity, the lifetime given by this approach is $\sim 10^7$ years. This compares favorably with a variety observational estimates of quasar lifetimes[23−26]. To cover the full range of uncertainty we consider modifications to our fiducial model in which the quasar lifetime is multiplied by a factor $f_{\rm lt}$ between 0.1–10, resulting in lifetimes for the observed quasars of $f_{\rm lt} t_{\rm lt} = 10^6$–$10^8$ years.

We have produced 300 realizations of the merger tree, and computed the evolution of the Strömgren sphere in each case for the full range of neutral fractions $0.001 \le x_{\rm HI} \le 1.0$, allowed by the Gunn-Peterson optical depth[1]. We find that quasar activity associated with the hierarchical build up of the host galaxy produces an H II region with a typical size of $\sim 2 x_{\rm HI}^{-1/3}$Mpc, comparable to the observed radii if $x_{\rm HI}$ is of order unity. Figure 1 shows the conditional a priori probability distributions of $R_{\rm p}$ for quasars like SDSS J1030+0524, assuming $x_{\rm HI} = 1$ and two different values of $f_{\rm lt}$. The observed radii are consistent with lifetimes close to the fiducial case of $f_{\rm lt} = 1$. The plotted distribution of $R_{\rm p}$ implies that the

hierarchical evolution of early quasars leads to a dearth of small Strömgren sphere radii for the *observed* SDSS quasars. This is in contrast to the simplified monolithic model of quasar formation[16,1], for which the H II region has zero volume at the time when the quasar turns on $[R(t_{\rm age}=0)=0]$ and the distribution extends down to $R_{\rm p}=0$.

To constrain the neutral fraction, we have computed the likelihood of observing $R_{\rm obs}=4.5$Mpc around SDSS J1030+0524 and $R_{\rm obs}=4.7$Mpc around SDSS J1148+5251 as a function of $x_{\rm HI}$ and $f_{\rm lt}$. The results are plotted in Figure 2. The upper panels show the locus of most likely values (thick line) as well as likelihood contours at 0.1 of the peak value (dashed lines). The fiducial lifetime ($f_{\rm lt}$) favors $x_{\rm HI}\sim 1$, while with $f_{\rm lt}\ll 1$ the distributions for $R_{\rm p}$ lie substantially below the observed value of 4.5Mpc, making smaller values of $x_{\rm HI}$ more likely. Extrapolation of the most likely contour for the Elvis et al.[19] template yields $f_{\rm lt}\sim 2x_{\rm HI}$. This implies that $x_{\rm HI}\sim 10^{-3}$ would require a lifetime as short as 2×10^4 years, which is ruled out by variability properties of quasars in SDSS[26]. The a posteriori probability distributions for $x_{\rm HI}$ given $f_{\rm lt}$ are plotted in the lower panels of Figure 2 and robustly yield the constraint $x_{\rm HI}\gtrsim 0.01$. For $f_{\rm lt}\gtrsim 0.3$, we find $x_{\rm HI}\gtrsim 0.1$ and $x_{\rm HI}\gtrsim 0.4$ at the 90% level for the Elvis et al.[19] and Telfer et al.[18] spectra, respectively. The fiducial model with $f_{\rm lt}=1$ yields corresponding constraints of $x_{\rm HI}\gtrsim 0.3$ and $x_{\rm HI}\gtrsim 0.6$.

The inference of a large neutral fraction at $z\sim 6.3$ presents a challenge to theories of cosmological reionization when combined with the large optical depth[3] to electron scattering after cosmological recombination, $\tau_{\rm es}=0.17\pm 0.04$. Consider a toy model in which the universe was partially reionized at a high redshift $z_{\rm reion,I}$, leaving a neutral fraction $x_{\rm HI}$ until complete reionization was reached at $z_{\rm reion,II}\sim 6.25$. The optical depth is then $\tau_{\rm es}=0.04+0.002(1-x_{\rm HI})\left[(1+z_{\rm reion,I})^{3/2}-19.5\right]$. If the IGM ionization fraction increased monotonically, then given $\tau_{\rm es}>0.13$, the universe needed to be reionized earlier than $z_{\rm reion,I}\sim 18$ or $z_{\rm reion,I}\sim 24$ assuming the Elvis et al.[19] and Telfer et al.[18] spectra,

respectively. If $\tau_{\rm es} = 0.17$ and $x_{\rm HI} > 0.7$, as implied by the Telfer et al.[18] spectrum, then a monotonic reionization history requires significant reionization at an implausibly high redshift ($z \geq 30$). In this case, a more plausible alternative is a non-monotonic history with an early reionization peak, possibly due to the formation of massive population-III stars[27,28].

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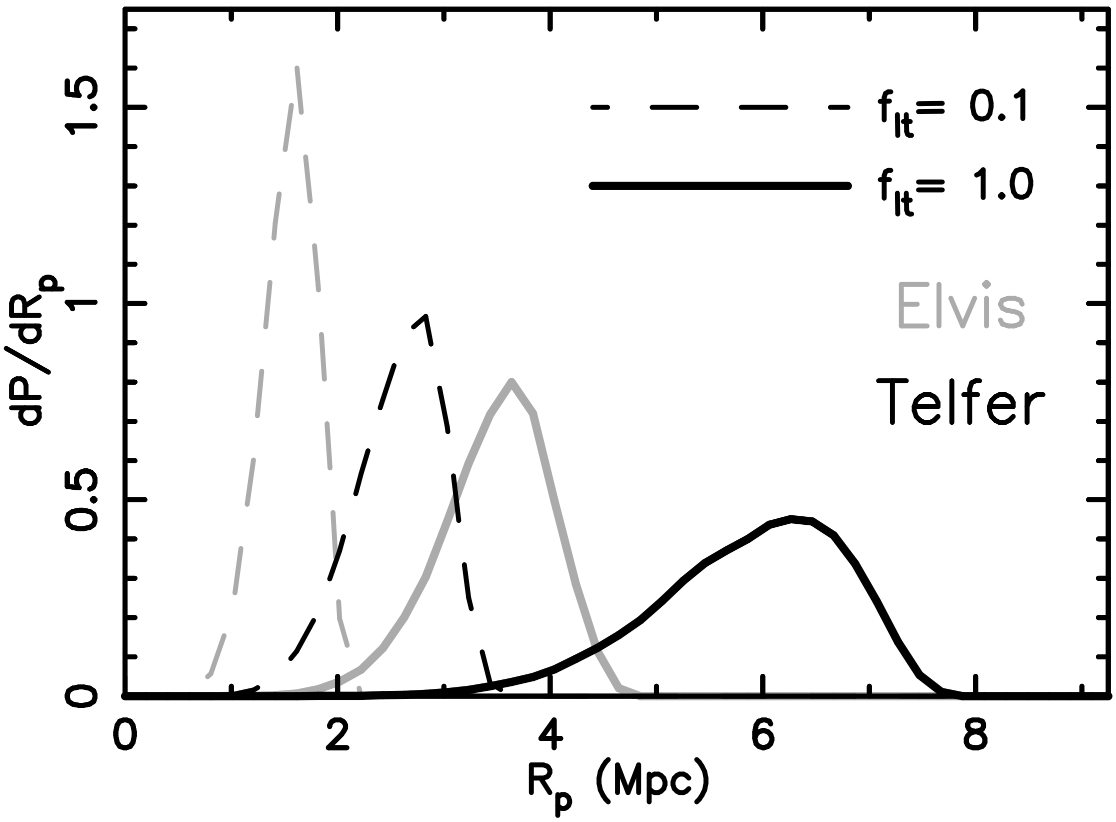
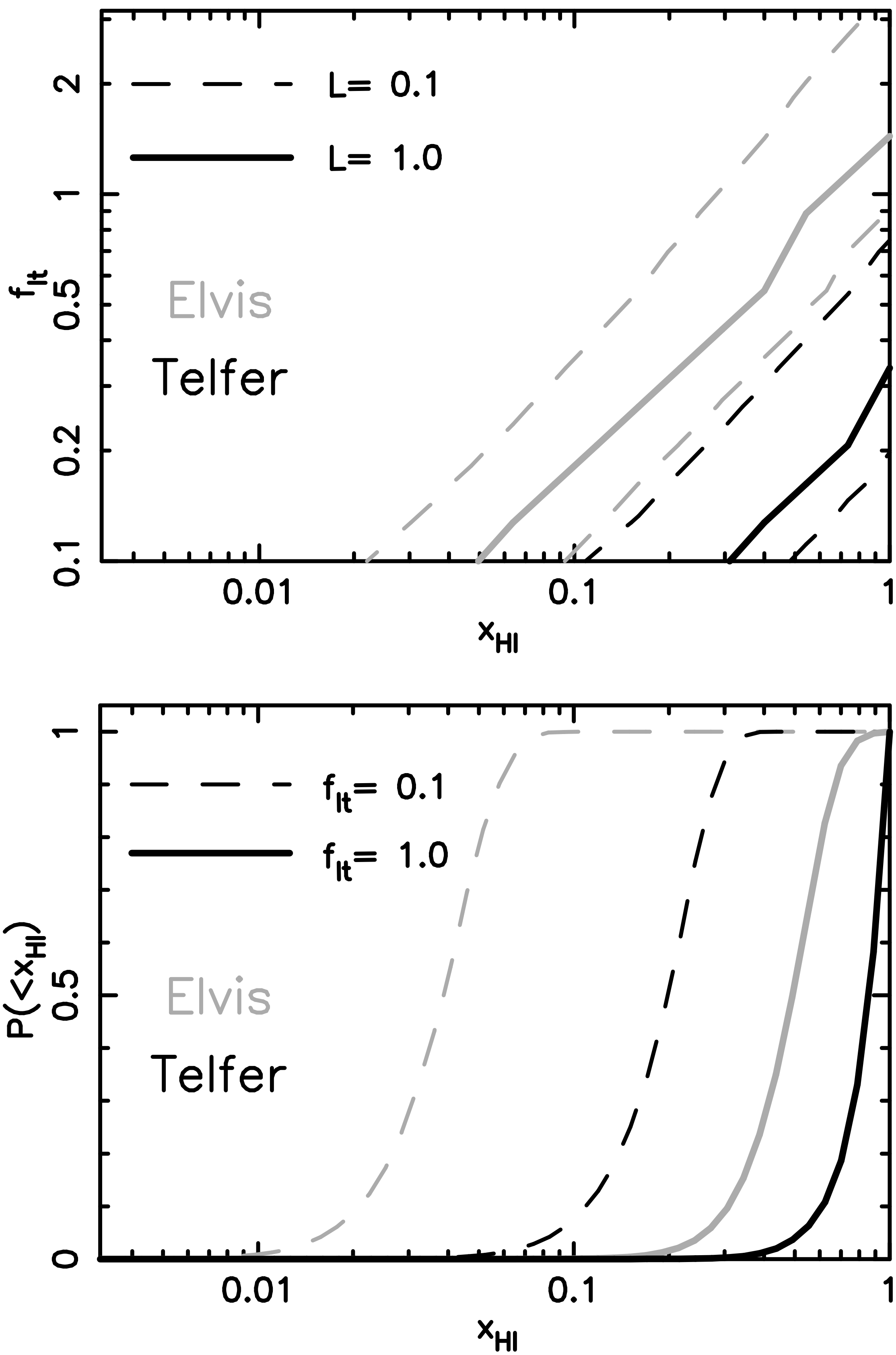
Fig. 1.— Predicted probability for observing different radii of the ionized region around the quasar SDSS J1030+0524. The differential a priori probability distribution is plotted for $x_{\rm HI} = 1$ and two quasar lifetimes: $f_{\rm lt} = 0.1$ (*dashed*) and $f_{\rm lt} = 1.0$ (*solid*). The *light* and *dark* curves show results calculated based on the Elvis et al.[19] and Telfer et al.[18] template spectra, respectively. The distributions may also be used to approximate the behavior with $x_{\rm HI} < 1$ by replacing $R_{\rm p}$ with $R_{\rm p} x_{\rm HI}^{-1/3}$. Values of $R_{\rm p}$ significantly larger than observed still allow transmission of Lyα flux at a detectable level because: (i) the optical depth due to the damping wing of the IGM[29] is only important near the boundary of the H II region, and (ii) the optical depth at $R_{\rm p}$ due to resonant absorption within the H II region[14] is in the range $\tau_{\rm reson} = (1-8) \times (R_{\rm p}/4.5~{\rm Mpc})^2$. A dense H I cloud near $R_{\rm obs}$ could produce a large damping wing and lead to a systematic underestimation of R_p. However, such a cloud would need a column density $\gtrsim 10^{21}\,{\rm cm}^{-2}$ ($\gtrsim 10^{22}\,{\rm cm}^{-2}$) to produce a Ly$\alpha$ optical depth > 26 over 10% (30%) of the spectral range covered by the H II region. This requires a damped Lyα absorber, whose existence is highly improbable within the narrow redshift interval under consideration, $\Delta z \sim 0.1$. Our calculation assumes that the ionization front is thin. The spectrum-averaged mean-free path for the ionizing quasar photons is $\lambda \sim 1.5 x_{\rm HI}^{-1}(1+z)^{-3}$Mpc, which may be compared to the bubble radius $R_{\rm p} \sim 4.5 x_{\rm HI}^{-1/3}$Mpc, to yield the fractional thickness of the ionization front $(\lambda/R_{\rm p}) \sim 10^{-3}\,(R_{\rm p}/4.5{\rm Mpc})^{-1}\,x_{\rm HI}^{-2/3}\,[(1+z)/7.3]^{-3}$. We also note that the ionized region need not be spherical; if the quasar radiation is beamed, its luminosity per unit solid-angle along the observer's line-of-sight is still measured, and equation (1) therefore describes the extent of the ionized region along the line-of-sight. Throughout our calculations, we have adopted the best-fit cosmological parameters derived from the WMAP data[30].



f_{lt}= 0.1
f_{lt}= 1.0
Elvis
Telfer
dP/dR$_p$
R$_p$ (Mpc)
0
0.5
1
1.5
0
2
4
6
8

Fig. 2.— Likelihood for the inferred neutral fraction of the IGM, assuming different quasar lifetimes. We show contours of likelihood, L, for $x_{\rm HI}$ and $f_{\rm lt}$ (*top*) and a posteriori cumulative probability distributions for $x_{\rm HI}$ (*bottom*). Cumulative distributions are shown for two different quasar lifetimes: $f_{\rm lt} = 0.1$ (*dashed*) and $f_{\rm lt} = 1.0$ (*solid*). The *light* and *dark* lines show results where the quasar ionizing photon rate was specified by the Elvis et al.[19] and Telfer et al.[18] spectra, respectively. The a posteriori probability is $\frac{dP}{dx_{\rm HI}}\Big|_{R_{\rm obs}} \propto \left[\frac{dP_{1030}}{dR_{\rm p}}\left(R_{\rm p} = 4.5{\rm Mpc}|\, x_{\rm HI}\right) \times \frac{dP_{1148}}{dR_{\rm p}}\left(R_{\rm p} = 4.7{\rm Mpc}|\, x_{\rm HI}\right)\right] \frac{dP_{\rm prior}}{dx_{\rm HI}}$, where $\frac{dP_{\rm prior}}{dx_{\rm HI}}$ is the prior probability for $x_{\rm HI}$, assumed to be flat in logarithmic bins within the range $0.001 \leq x_{\rm HI} \leq 1.0$, and $\frac{dP_{1030}}{dR_{\rm p}}$ and $\frac{dP_{1148}}{dR_{\rm p}}$ are the a priori probability distributions for $R_{\rm p}$ in quasars like SDSS J1030+0524 and SDSS J1148+5251, respectively. A flat logarithmic prior is the natural choice for $\frac{dP_{\rm prior}}{dx_{\rm HI}}$, because $x_{\rm HI}$ may be thought of as a ratio of independent quantities (the number of ionizing photons and the number of baryons) that would themselves have linearly distributed prior probabilities. The alternative use of a linear prior in $x_{\rm HI}$ leads to more stringent limits than those presented here.


L= 0.1
L= 1.0
Elvis
Telfer
f_{lt}
0.1
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x_{HI}
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Elvis
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